RAPID SIMULATION OF BOREHOLE NUCLEAR MEASUREMENTS
WITH APPROXIMATE SPATIAL FLUX-SCATTERING FUNCTIONS

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ABSTRACT

The Monte Carlo method has been the foremost numerical technique used to simulate borehole nuclear measurements. This is due to its detailed geometrical capabilities, high numerical accuracy, and ability to incorporate specific tool configurations and complex spatial distributions of material properties. Although recent advances in computer technology have considerably reduced the computer time required by Monte Carlo simulations of borehole nuclear measurements, the efficiency of the method is still not sufficient for either inversion techniques or joint interpretation with other borehole measurements.

We develop and benchmark fast approximate numerical procedures to simulate neutron and density porosity logs making use of Monte Carlo-derived spatial flux-scattering functions (FSFs) for specific nuclear tool configurations. To this end, we describe the flux at detectors due to particles emitted by the radioactive source with the integral representation of Boltzmann’s transport equation. Subsequently, we use the Monte Carlo Code MCNP to calculate the associated Green’s function and the background particle flux included in the integral form of the transport equation. The solution of the integral equation is approximated with a Born series expansion that includes various orders of interaction between material properties and sources in the calculation of particle flux.

Simulations performed with the new approximations entail percent errors of less than 10% with respect to Monte Carlo-simulated nuclear logs. Moreover, for the case of density FSFs we observed a maximum shift in the radially-integrated radial length of investigation (radial J-functions) of 0.3 inches due to variations of formation density. For the case of neutron FSFs the maximum change in the radial length of investigation due to variations of modified migration length was approximately equal to 2 inches. The approximations introduced in this paper enable the simulation of borehole nuclear measurements in seconds of CPU time compared to several days of CPU time with MCNP.

INTRODUCTION

A fast numerical method is essential to simulate nuclear borehole measurements in conjunction with inversion techniques as well as for their quantitative integration with other borehole measurements. This is not currently done for nuclear measurements, such as neutron and active gamma ray, mainly because of the implicit high computational requirements. For nuclear log simulations, the Monte Carlo method has been the most widely used approach because of its high numerical precision and detailed three-dimensional (3D) geometrical capabilities. However, the Monte Carlo method is not efficient neither for the application of inversion techniques (Patchett and Wiley, 1994) nor for the quantitative integration of nuclear measurements with other well logs. The particular case of logging while drilling (LWD) logs in high-angle wells, that entail simulations over long depth intervals and multiple azimuthal quadrants, is an example of the pressing need for fast forward numerical simulation of borehole nuclear measurements. Numerical simulation of nuclear measurements has been widely used to quantify environmental and petrophysical effects on borehole measurements. In addition, the Monte Carlo method has been extensively used to quantify effects of porosity and invasion on nuclear measurements (Ellis et al., 2003, 2004; Ellis and Chiaramonte, 2002; Mendoza et al., 2007). The same method has been used to quantify geometrical effects in nuclear measurements due to laminations in high-angle and horizontal wells (Mendoza et al., 2006; Yin et al., 2006; Radtke et al., 2007).

Watson (1984) introduced the concept of Monte Carlo-derived differential sensitivity functions for detector responses due to Compton and photoelectric gamma-ray interactions. This technique not only provided important information for tool design and improved post-processing of measured single-detector responses, but it opened the door to fast nuclear log simulation with the use of linear sensitivity functions. In addition, Aristodemou et al. (2006) developed a method to reduce the computational time required in the simulation of well-logging nuclear measurements using the concept of energy group optimization.
In this paper, we develop new linear and nonlinear fast numerical procedures to simulate nuclear well logs making use of spatial flux-scattering functions (FSFs) derived with the Monte Carlo method in a similar way to the sensitivity calculations described by Watson (1984, 1992), Couët and Watson (1992, 1993), and Case et al. (1994). Our objective is to approximate nuclear measurements acquired across layered formations with spatial distributions of a wide range of material property contrasts (cross-section, migration length, mass density, porosity, and fluid saturation) via linear first-order Born and Rytov approximations. In addition, we make use of the nonlinear extended Born approximation to simulate neutron measurements acquired in the presence of high contrasts of material properties.

We describe the basic physical parameters involved in our approximation technique starting with the solution of the integral form of Boltzmann’s transport equation (Tittman and Wahl, 1965). The formulation includes an overview of nuclear particle transport processes and identifies the geometrical properties of the model. We describe the basic components of Monte Carlo-derived spatial FSF approximations, and validate the formulation by comparing the corresponding simulation of particle flux at the detector calculated with MCNP (X-5 Monte Carlo Team, 2003). The approximations of neutron porosity and density measurements described in this paper are adapted from the extended Born approximation for the simulation of electromagnetic borehole measurements introduced by Torres-Verdín and Habashy (2001). To quantify the FSFs in the presence of changes in the total cross-section of the material, we perform a sensitivity analysis over a wide range of porosity values and rock matrix types. In addition, we quantify the effect of spatial variation of neutron FSFs due to a boundary between two formations of contrasting porosities. Finally, we describe numerical results for the approximation of neutron and density measurements with the use of the FSFs. To benchmark these approximations, we compare fast simulation results against synthetic nuclear logs calculated with MCNP. Simulations include the cases of vertical and radial variations of formation properties. The adaptation of the FSF approximations to the rapid simulation of nuclear logs in highly-deviated wells (which entails simultaneous variations in the vertical and horizontal direction) is currently under development.

FORMULATION

To introduce terminology, and to describe the general formulation of the approximations introduced in this paper, we begin with a formal description of nuclear particle transport via Boltzmann’s equation, given by

\[ \Omega \cdot \nabla \Phi(r,E,\Omega) + \Sigma \Phi(r,E,\Omega) = \int dE \int d\Omega \Sigma_s(r,E,\Omega,\Omega') \Phi(r,E',\Omega') + q(r,E,\Omega), \]

(1)

where \( \Phi \) is the angular particle flux at position \( r \) of energy \( E \) and direction \( \Omega \), \( \Sigma \) is the total macroscopic cross-section, \( \Sigma_s \) is the macroscopic scattering cross-section, and \( q \) is the source (refer to Appendix A for further details on the above equation). The counting rate at each detector due to a radioactive particle source is influenced by the material properties of the formation (Ellis, 1987). We approximate the flux at the detectors assuming a background medium of constant cross-section \( \Sigma_b \) and \( \Sigma \) variations away from the homogenous background using the concept of superposition. The estimated flux at the detector location \( r_s \) in a non-homogeneous formation can then be written as

\[ \Phi(r_s,E) = \Phi_b(r_s,E) + \Delta \Phi(r_s,E), \]

(2)

where \( \Delta \Phi(r_s,E) \) is the secondary flux at the detector due to a variation of \( \Sigma \) in the formation, i.e., \( \Delta \Sigma = \Sigma_b(r,E) - \Sigma(r,E) \). The function \( \Phi_b(r_s,E) \) is the flux at the detector due to the assumed background formation, and is given by

\[ \Phi_b(r_s,E) = \int dE \int d\Omega \left( \int dE' \int d\Omega' \Sigma_b(r,E',\Omega',\Omega) \right) \Phi_b(r_s,E',\Omega'). \]

Fig. 1 Schematic diagram of the geometrical components of the nuclear logging tool, borehole, and formation model considered in the general formulation. We assume neutron and density tool models consisting of short- (near) and long-spaced (far) detectors at locations \( R_2 \) and \( R_1 \), respectively, and a radioactive source located at \( S \). The particle flux at each detector is given by \( \Phi_b(r_s,E) \) whereas the point source at \( S \) is described by \( q(r_s,E) \).
\[ \Phi_\beta (r_\beta) = \int_{E_b}^{E_c} \int dE \int d\Omega \]

\[ \cdot \int \mathbf{G}(r, E, \Omega \to r', E, \Omega) \Phi_\beta (r, E, \Omega) d\mathbf{r}, \]  

(3)

where \( \Phi_\beta (r, E, \Omega) \) is the differential background flux, \( \Phi_\beta (r_\beta) \) is the scalar background flux at the detector, and \( \mathbf{G}(r, E, \Omega \to r', E, \Omega) \) is Green’s function (Greenspan, 1976). Appendix A provides further details about the above equations.

Figure 1 illustrates the geometrical and formulation conventions. We assume a homogeneous background, \( \mathcal{K} \), of known cross-section, \( \Sigma_b (r, E) \), and a scatterer region, \( \mathcal{K} \), of cross-section \( \Sigma(r, E) \). The position vector \( \mathbf{r} \) is a function of the radial direction \( \rho \), and the vertical location, \( z \). Formation properties are axial-symmetric about the axis of a vertical well. We assume an 8-inch borehole, and two-dimensional (2D) axial-symmetric media about the axis of the well.

**SCATTERING APPROXIMATIONS**

At the outset, we describe linear and nonlinear approximations of the FSFs for the rapid simulation of nuclear borehole measurements. We consider the Born and Rytov approximations, and the extended Born approximation in analogy with that introduced by Torres-Verdín and Habashy (2001) for electromagnetic scattering. Subsequently, we describe and benchmark a technique for calculating FSFs with MCNP.

**Born Approximation.** In Equation (2), the secondary flux at the detector is approximated by

\[ \left\{ \frac{\Delta \Phi (r_\beta)}{\Phi_\beta (r_\beta)} \right\} \cong \ln \left[ \Phi (r_\beta) \right] - \ln \left[ \Phi_\beta (r_\beta) \right], \]

Equation (2) can be approximated as

\[ \Phi (r_\beta) \cong \Phi_\beta (r_\beta) \exp \left( \frac{\Delta \Phi (r_\beta)}{\Phi_\beta (r_\beta)} \right), \]

(6)

where \( \Delta \Phi (r_\beta) \) is given by Equation (4).

**Extended Born Approximation.** In the case of large formation-property contrasts between the scattering medium and the assumed background, or when the scattering medium is located in close proximity to the radioactive source, an auxiliary function \( Y(r) \) is convenient to describe the scattered flux. It follows that

\[ Y(r) \equiv \Phi_\beta (r) \left[ \Phi_\beta (r) - \int_{E_i}^{E_1} dE \right. \]

\[ \left. \cdot \int \mathbf{G}(r_0, E \to r_0', E') \Phi_\beta (r_0, E') \frac{\Delta \Sigma (r_0, E)}{\Sigma_b (r_0, E)} d\mathbf{r}_0 \right]^{-1}, \]

whereupon the corresponding FSF is given by

\[ \Phi_b (r_\beta, E) = \mathbf{G}(r_0, E \to r_\beta, E) \Phi_\beta (r_0, E) Y(r_0). \]

(7)

Appendix B provides further details about the above expressions.

With the use of the Monte Carlo code MCNP, we calculate the spatial flux \( \Phi_\beta (r, E) \) in the formation due to a specified source distribution in a homogeneous background medium (which includes the borehole). Furthermore, for each neutron and gamma ray detector, we calculate the corresponding response given by the Green’s function \( \mathbf{G}(r, E \to r_\beta, E) \), with the use of the forward-adjoint generator implemented in MCNP to calculate space and energy-dependent weight windows (Booth and Hendricks, 1984; Hendricks, 1992). Moreover, we modify the MCNP code to optimize the calculation of the FSF with the use of a superimposed geometry to reduce the input of a fine spatial grid, and to render the FSF as a direct output of an MCNP run. Finally, to further improve the efficiency of the calculations, we implement a modification of MCNP that automatically updates the generated weight windows and more rapidly converges to the optimum detector response.

To illustrate the calculation of the FSF, Figure 2 shows the one-dimensional (1D, vertical direction) graphical...
spatial functions involved (background flux and Green’s function) in the calculation of the FSF for the case of a neutron far detector. Figures 3 and 4 show normalized FSF maps of density and neutron measurements, respectively. For density measurements, we calculate separate FSFs for Compton (density) and photoelectric effect (PEF). For the case of neutron FSFs, we include all neutron energies. Figure 4 indicates that the neutron FSF exhibits a more pronounced peak in the vicinity of the detector than in the vicinity of the source. This behavior remains consistent with the neutron sensitivity functions calculated by Couët and Watson (1993). By comparison, Figure 3 shows a more symmetric FSF for the case of density measurements.

To quantify the accuracy of the density and neutron FSFs, we compare the flux at each detector calculated via the flux tally in MCNP against the scalar flux calculated with the integral of the corresponding FSF (Equation 3). In so doing, we assume a variable background flux at each depth sample point.

Figure 5 compares numerical simulations of the gamma-ray flux for Compton scattering measured at the long-spaced (LS) detector across a boundary between 0 and 10% porosity water-filled sandstone. The accuracy of the Monte Carlo calculations is no worse than 1%. On the other hand, the percent difference between the counting rate at the detector simulated with the standard MCNP flux tally and the one simulated with the integral of the FSF is within 5%, which corresponds to differences in bulk density of approximately ±0.016 g/cm³. We observe comparable results for the case of the short-spaced (SS) detector. Figure 6 describes a similar comparison for the case of the near and far detectors of the neutron measurement.
Fig. 5  Comparison of the gamma-ray flux and the spatial integral of the density FSF. The solid line in the left panel describes the MCNP-calculated gamma ray flux at the LS detector across a boundary between two formations of contrasting petrophysical properties. The blocky line identifies the gamma-ray flux at the detector calculated with the spatial integral of the corresponding density FSF at each sample point. The right panel describes the percent difference between the two calculations.

Fig. 6  Comparison of the neutron flux and the spatial integral of the neutron FSF. Solid lines describe the MCNP-calculated neutron flux at the detectors across three formation layers of contrasting petrophysical properties. Blocky lines identify the neutron flux at the detector calculated with the spatial integral of the corresponding FSF at each sample point.

Sensitivity of the FSF to Formation Properties. The principle behind the rapid simulation of nuclear borehole measurements with Equations (4) and (6), is to assume a constant background (which includes the borehole) for the calculation of the FSFs. Since the FSF weighs spatial variations of formation properties (cross-section, mass density, migration length, porosity) to approximate the corresponding variation of detector response, the spatial properties of the FSF are critical to the simulations. Therefore, to appraise the performance of FSFs for different choices of background, we calculate FSFs for density and neutron measurement for a wide range of homogeneous formations.

Figure 7 describes the spatial sensitivity of the density-measurement FSF to formation density. In the vertical direction, we observe that the maximum variation occurs in the vicinity of the source and the detector. In addition, the maximum variation is approximately 10% for the LS detector, and less than 5% for the SS detector. Similarly, in the radial direction, the radial J-functions show a maximum variation of approximately 0.3 inches for 80% of the response at the LS detector, and much smaller for the case of the SS detector.

Fig. 7  Spatial sensitivity of the density FSF to formation mass density for the SS and LS detectors. Panels on the left describe normalized 1D FSFs (integrated in the radial direction) of the SS and LS detectors of a density tool. Panels on the right are similar 1D plots of the radial J-functions of the FSF. Colored curves describe FSFs for several homogeneous formations of a wide range of mass density values. The vertical red line identifies the approximate location of the radioactive source, and vertical black lines indicate the detector position. Refer to Figure 1 and Table 1 for additional details of source-sensor conventions and formation properties.

Figure 8 describes the spatial sensitivity of the neutron-measurement FSF to the formation modified migration length. In the vertical direction, maximum variations occur in the vicinity of the source and detector. Moreover, the total FSF variation is as large as 60% for the far detector, and as large as 45% for the near detector. In the radial direction, the J-functions exhibit a maximum variation of approximately 2 inches for 80% of the response of the far detector, and 1.5 inches for the case of the near detector.
Fig. 8  Spatial sensitivity of neutron FSF to formation modified migration length for the near and far detectors. Panels on the left describe normalized 1D FSFs (integrated in the radial direction) of the near and far detectors of a neutron tool. Panels on the right are similar 1D plots of the radial $J$-functions of the FSF. Colored curves describe FSFs for several homogeneous formations of a wide range of migration length values. The vertical red line identifies the approximate location of the radioactive source, and vertical black lines indicate the detector position. Refer to Figure 1 and Table 1 for additional details of source-sensor conventions and formation properties.

Table 1- Composition in percent volume and properties of the materials in the homogeneous formation models used to calculate the density and neutron flux-scattering functions (FSFs) described in Figures 7 and 8.

<table>
<thead>
<tr>
<th>Reference Formation</th>
<th>Composition [%]</th>
<th>Density [g/cm$^3$]</th>
<th>PEF [b/e]</th>
<th>$\mu^*$ [cm]</th>
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</thead>
<tbody>
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<td>Form 1</td>
<td>35 H$_2$O + 65 SiO$_2$</td>
<td>2.0725</td>
<td>1.54</td>
<td>11.91</td>
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<tr>
<td>Form 2</td>
<td>25 H$_2$O + 75 SiO$_2$</td>
<td>2.2375</td>
<td>1.63</td>
<td>14.10</td>
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<td>Form 3</td>
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<td>2.4025</td>
<td>1.71</td>
<td>18.07</td>
</tr>
<tr>
<td>Form 5</td>
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<td>21.61</td>
</tr>
<tr>
<td>Form 6</td>
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<td>1.77</td>
<td>27.81</td>
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<tr>
<td>Form 7</td>
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<td>34.87</td>
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<tr>
<td>Form 8</td>
<td>35 CH$_4$ + 65 SiO$_2$</td>
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<td>1.79</td>
<td>46.93</td>
</tr>
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<td>38.25</td>
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RAPID SIMULATION OF NUCLEAR MEASUREMENTS: NUMERICAL RESULTS

In this section we describe numerical results obtained for the simulation of neutron, density, and photoelectric factor (PEF) measurements performed with the approximations described above. Appendix C provides additional details about the specific mathematical expressions used to perform the simulations.
source-detector spacing) and the midpoint between the source and detector is equivalent for the near and far detectors. For those cases where the boundary is near one end of the tool, we observe limited variation in the FSF regardless of the location of the low- and high-porosity formations. However, when the boundary is near the midpoint between source and detector, the formation around the detector dominates the value of porosity. Moreover, the FSF exhibits a spatial distribution approximately equal to that of the corresponding FSF of a homogeneous background corresponding to the average formation property around the detector.

Results shown in Figures 8 and 9 indicate that, when used for a fast simulation of a neutron log across a layered formation, the spatial neutron FSF must be modified from that of a starting background formation to one of similar properties of the adjacent bed. Accordingly, the extended Born approximation adjusts the neutron FSF, calculated for an assumed background, to one corresponding to a reference formation. Figure 10 describes a FSF calculated with the extended Born approximation for the case of the far neutron detector.

We choose the modified migration length as the appropriate weighed parameter in Equation (C1) because it retains dependence on material cross-section (Ellis et al. 1987). With the use of this equation, we simulate the near- and far-detector responses across a boundary between water-filled sandstone formations of 5 and 10% porosity (Figure 11). For this particular contrast, the change in detector response as a function of the inverse modified migration length is linear and hence, Equation (C1) yields an accurate approximation with a difference within 5% with respect to the same neutron log simulated with the Monte Carlo method. The FSF assumed a constant homogeneous background corresponding to the 5%-porosity formation. Similar results were obtained when choosing a constant homogeneous background corresponding to the 10%-porosity formation. For this particular case, the Monte Carlo simulations required 700 minutes of CPU time (for 25 sample points and 2 detectors) while the FSF approximation (without considering the time involved in calculating the FSF) required 53 seconds of CPU time.

**Density and PEF Measurements.** For the case of rapid simulation of density measurements via the Born approximation (Equation C1), we choose the electron density of the formation as the weighed property. Alternatively, for the calculation of PEF we use the Rytov approximation (Equation C4). Figure 12 compares numerical simulations performed with the rapid FSF approximation and the Monte Carlo method for the case of periodic 4-inch thick beds of density values equal to 2.0 g/cm$^3$ and 2.6 g/cm$^3$. The FSF approximation yields a maximum difference of 0.012 g/cm$^3$ for the filtered SS detector density, and of 0.008 g/cm$^3$ for the depth-matched LS detector density.

**Fig. 10** Extended Born approximation of the neutron FSF. The dotted blue line describes the neutron FSF for a background water-saturated sandstone formation of 5% porosity, the dashed black line identifies a reference formation of 30% porosity water-saturated sandstone, and the solid red line is the approximation to the reference formation with the use of Equation (7). The top panel shows the approximation in absolute flux terms, and the bottom panel shows the spatial FSF normalized with respect to the maximum value in the vicinity of the detector.

**Fig. 11** Comparison of the FSF approximation and Monte Carlo simulations of a neutron log across a boundary between two formations of moderate contrast of modified migration length. Solid red lines describe the rapid FSF approximation, and dashed black lines describe the Monte Carlo simulation. The left and central panels describe the far- and near-detector responses, respectively, whereas the right panel shows the corresponding neutron porosity.
Fig. 12  Comparison of the FSF approximation and Monte Carlo simulations of density measurements across periodic 4-inch layers of mass densities equal to 2.0 g/cm$^3$ and 2.6 g/cm$^3$. Solid red lines describe the rapid FSF approximation, and dashed black lines identify the Monte Carlo simulations. Left-hand panels describe simulations of the raw single-detector measurements and the standard compensated density. The solid blue line describes the difference in compensated density between the FSF approximation and the Monte Carlo. The right-hand panels show the simulated photoelectric and volumetric photoelectric factors. Dark and white blocks identify the higher- and lower-density materials, respectively. The FSF approximations for the case of density were calculated with the Born approximation (Equation 4), and the cases of PEF and $U$ were calculated with the Rytov approximation (Equation 6). The FSF approximation assumes a homogeneous background of mass density equal to 2.6 g/cm$^3$.

Fig. 13  Comparison of the FSF approximation and Monte Carlo simulations of density measurements across a wide range of mass density and bed-thickness values. Solid red lines describe the rapid FSF approximation, and dashed black lines identify the Monte Carlo simulations. The FSF approximations of density measurements were calculated with the Born approximation (Equation 4). Refer to Table 2 for additional details on formation model properties. The FSF approximation assumes a homogeneous background of mass density equal to 2.6 g/cm$^3$. 
After post-processing of the single-detector responses, the compensated density exhibits a maximum difference of 0.018 g/cm³ between the rapid FSF approximation and the Monte Carlo simulation. Similarly, for the volumetric photoelectric factor (U) comparison between the rapid FSF and the Monte Carlo simulation indicates a maximum difference of 0.2 b/cm³ (PEF was derived from the simulated U).

To quantify the accuracy of the rapid FSF density and PEF simulations, with respect to those yielded by the Monte Carlo method, under variable bed-thickness and density contrasts, we simulate the SS and LS detector density measurements across the complex formation model described in Figure 13 and Table 2.

<table>
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<th>Layer</th>
<th>Thickness [in]</th>
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<th>PEF [b/e]</th>
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</table>

For the results shown in Figure 13, the FSF approximation assumed a homogeneous background of 2.6 g/cm³ across the entire depth interval. We approximate Monte Carlo-simulated raw single-detector measurements and subsequently apply conventional density post-processing. The accuracy of the FSF approximation for this case is comparable to that of the results shown in Figure 12. For this particular example, Monte Carlo simulations required approximately 154,000 minutes of CPU time for 275 sample points and 2 detectors. By contrast, the density measurements simulated with the FSF approximation method required 56 seconds of CPU time (without considering the CPU time required to calculate the FSF).

To quantify the accuracy of the rapid density simulation method for the case of formation property variations in the radial (horizontal) direction, we consider the case of two materials with a large contrast in mass density. Figure 14 shows LS-detector simulations for the case of a formation of density equal to 2.60 g/cm³, and an axial-symmetric water layer (density equal to 1.00 g/cm³) of several values of radial distance measured from the borehole wall. All remaining formation properties are kept constant in the vertical direction. For the particular case of a thin layer of water around the borehole (tool standoff or mudcake), in the proximity of the source and detector, we observe a substantial change in the spatial shape of the FSF. This behavior is due to the tendency of gamma rays to channel through the water layer. With the use of a FSF with the spatial shape shown in Figure 14, and Equation (C1), we approximate the Monte Carlo-calculated values of density for increasing values of radial thickness of the water layer. Simulation results indicate differences of less than 0.02 g/cm³ up to 3 inches of water in the radial direction from the borehole wall with the use of the constant FSF shown in Figure 14.
**Spontaneous Gamma-Ray Measurements.** In addition to neutron and density measurements, the FSF calculation technique described in this paper can be applied to the derivation of natural gamma-ray FSFs. In the case of natural gamma-ray measurements, the background flux in Equations (5) and (7) is due to a volume-distributed radioactive source in the formation instead of a point source inside the logging tool. To illustrate this situation, we define a uniform volume-distributed radioactive source for unit concentrations of Thorium, Uranium, and Potassium (Mendoza et al., 2006), and calculate the corresponding FSF. Figure 15 shows the natural gamma-ray FSF for a hypothetical NaI detector located inside the borehole.

![Image](image_url)

**Fig. 15** Flux-scattering function associated with natural gamma-ray measurements. The top-left panel shows the 2D plot of the gamma-ray detector response. Top-right and bottom panels show the corresponding 1D plots along the axis of the borehole and the radial J-function, respectively.

**SUMMARY AND CONCLUSIONS**

We described a new numerical method to calculate spatial flux-scattering functions with the Monte Carlo code MCNP. In so doing, we used first-order Born, first-order Rytov, and nonlinear extended Born approximations for the rapid simulation of neutron, density, and photoelectric factor measurements.

Results indicate that the FSFs calculated with the technique described in this paper accurately reproduce the particle flux calculated with a conventional Monte Carlo flux tally with a precision of less than 5%. In addition, sensitivity analyses of the FSFs for a wide range of formations properties confirmed that the density FSF is much less affected by variations of formation properties than the neutron FSF. Therefore, we made use of the extended Born approximation to modify the neutron spatial FSF thereby considerably improving the accuracy of the neutron flux approximation.

For the case of rapid simulation of density measurements, assuming a spatial FSF derived for a homogeneous background, the approximations entailed differences of less than 0.02 g/cm³ with respect to density measurements simulated with the Monte Carlo method. Similar results were observed for the case of neutron measurements across formations with small differences of modified migration length. For cases of larger contrast of material properties, the relationship between variations of modified migration length with respect to a change of particle flux at the detector is highly nonlinear. Therefore, the FSF used in the rapid simulation must be locally adjusted to a FSF associated with an equivalent (average) local background.

For simulations of nuclear measurements over a given depth interval (that requires numerous sample points) the rapid simulation based on FSF approximations can reduce CPU time from several days with Monte Carlo calculations, to seconds.

The FSF approximations enable the accurate and the rapid simulation of nuclear density and neutron porosity wireline and LWD measurements. Moreover, this technique can be applied to simulate gamma-ray, thermal neutron decay, and nuclear spectroscopy logs. There may be special cases such as unique minerals or geometries that would require a Monte Carlo calculation to generate a new set of FSFs. Future work will incorporate the effects of key borehole-environmental properties such as mudcake for the density tool, and standoff for the neutron tool. In addition, the FSF simulation technique allows one to reproduce nuclear measurements for a wide range of rock formation properties without requiring proprietary nuclear tool design information. Nuclear tool design information is only required to generate the FSFs.

**NOMENCLATURE**

- \( C_N \) Coefficient for neutron approximation [ ].
- \( C_{PE} \) Coefficient for PEF approximation [ ].
- \( C_p \) Coefficient for density approximation [ ].
- \( E \) Energy of the incoming particle [eV].
- \( E' \) Energy of the scattered particle [eV].
- \( L_{d} \) Diffusion length [cm].
- \( L_{m} \) Modified migration length [cm].
- \( L'_{m,b} \) Modified migration length of the background medium [cm].
$L_s$ Slowing-down length [cm].

$PEF$ Photoelectric factor [b/e].

$q$ Source at $r$ of energy $E$ and direction $\Omega$ [particles/sh].

$r_s$ Position vector inside a scatterer region of $\Sigma(r_s, E) \neq \Sigma_0(r, E)$.

$r$ Position vector in space.

$R$ Observation point (detector position).

$S$ Point-source position.

$U$ Volumetric photo electric factor. $U=\rho \cdot PEF$ [particles/cm$^3$].

$v$ Particle velocity vector [cm/sh].

$z$ Vertical direction.

$\Delta \Sigma$ Excess background total macroscopic cross-section for all interactions of particles of energy $E$ at $r$ [1/cm].

$\Psi$ Angular density. Expected number of particles at $r$ of energy $E$ and direction $\Omega$ [particles/cm$^3$].

$\lambda_0$ Mean free path (average distance a neutron will travel before undergoing a particular interaction) [cm].

$\Omega$ Unit direction of incoming particles.

$\Omega'$ Unit direction of scattered particles.

$\Phi$ Angular flux at $r$ of energy $E$ and direction $\Omega$ [particles/cm$^2$-sh].

$\Phi_B$ Background angular flux at $r$ of energy $E$ and direction $\Omega$ [particles/cm$^2$-sh].

$\rho$ Radial direction.

$\rho_e$ Electron density [g/cm$^3$].

$\Sigma$ Secondary total macroscopic cross-section for all interactions of particles of energy $E$ at $r$ [1/cm].

$\Sigma_a$ Macroscopic absorption cross-section for particles of energy $E$ at $r$ [1/cm].

$\Sigma_B$ Total macroscopic cross-section of the background for all interactions of particles of energy $E$ at $r$ [1/cm].

$\Sigma_s$ Macroscopic scattering cross-section for particles of energy $E$ at $r$ [1/cm].

$\Sigma_t$ Total macroscopic cross-section for all interactions of particles of energy $E$ at $r$ [1/cm].

$v$ Particle speed [cm/sh].

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**APPENDIX A: Background Theory**

The well-known Boltzmann transport equation in its time-independent, one-speed form is written as (Glasstone, 1994)

\[
\Omega \cdot \nabla \Phi(r, E, \Omega) + \Sigma_{i} \Phi(r, E, \Omega) = \\
\frac{d\Omega}{dE} \int dE \Sigma_{\nu} \Phi(r, E, \Omega) \\
\frac{d\Omega}{dE} \int dE \Sigma_{\nu} \Phi(r, E, \Omega) \\
\frac{d\Omega}{dE} \int dE \Sigma_{\nu} \Phi(r, E, \Omega) \\
\frac{d\Omega}{dE} \int dE \Sigma_{\nu} \Phi(r, E, \Omega)
\]

where \( \Phi(r, E, \Omega) = \nu \Psi(r, E, \Omega) \), \( \Omega = \frac{v}{\nu} \), \( \nu = |v| \), and \( \Sigma_{i} = \Sigma_{a} + \Sigma_{s} = \frac{1}{\lambda_{nu}} \).

The terms included in Equation (A1) have the following physical meaning:
I Rate of loss of particles of energy \(E\) and direction \(\Omega\) from volume element at \(r\) as a result of leakage,

II Rate of loss of particles of energy \(E\) and direction \(\Omega\) from volume element at \(r\) as a result of nuclear interactions of all types.

III Rate of gain of particles of energy \(E\) and direction \(\Omega\) from the volume element at \(r\) as a result of nuclear interactions of particles with all initial energies and directions, and

IV Gain of particles of energy \(E\) and direction \(\Omega\) from the volume element at \(r\) from a source.

Borehole nuclear measurements are best described with the particle flux at the detectors, \(\Phi(r_s,E,\Omega)\), given by the solution of Equation (A1).

For the formulation described in Figure 1, in the presence of a scatterer region with \(\Delta \Sigma(r,E) = \Sigma(r,E) - \Sigma_a(r,E)\), the solution of Equation (A1) can be written as

\[
\Phi(r_s,E) = \Phi_a(r_s,E) + \Delta \Phi(r_s,E), \tag{A2}
\]

where \(\Phi(r_s,E)\) is the total particle flux at the detector position \(r_s\), \(\Phi_a(r_s,E)\) is the primary flux in a volume element at \(r_s\) due to a source \(q(r_s,E)\) in a medium of macroscopic cross-section equal to \(\Sigma_a(r,E)\), and \(\Delta \Phi(r_s,E)\) is the secondary flux (positive or negative) in a volume element at \(r_s\) due to a source \(q(r_s,E)\) and a non-zero \(\Delta \Sigma(r,E)\) in the volume inside the scatterer region \(\mathcal{S} \subset \mathbb{R}^3\).

**Green's Function.** The Green’s function describes the particle flux due to a single scattering point (concentrated source) in the system. The solution of \(\Phi(r,E)\) for the case of an infinite medium of constant cross-section due to an infinitesimal point source is given by \(G(r,E \rightarrow r_s,E)\), where \(r_s\) and \(E\) are the location and energy of the source, respectively. Because of linearity, the solution of the transport equation for any given point \(r\) can be expressed as a superposition of basic solutions (Case, 1967). Accordingly, the detector response distribution function \(G(r,E \rightarrow r_s,E)\) can be defined as the contribution made by one material source located at \(r\) to the flux measured at the detector. Thus, the solution to the transport equation can be expressed with two functions, the flux \(\Phi(r,E)\) within the scattering medium and its importance for a detector reading \(G(r,E \rightarrow r_s,E)\) (Lewins, 1965; Greenspan, 1976). In so doing, the total particle flux at the detector \(\Phi(r_s,E)\) is equal to the sum over all \(\Phi(r,E)\) each weighted by its contribution to the detector reading, namely,

\[
\Phi(r_s,E) = \int_{E_l}^{E_u} dE \int d\Omega \cdot \int_{\mathcal{S}} G(r,E \rightarrow r_s,E,\Omega) \Phi(r,E,\Omega) \, dr.
\]

**APPENDIX B: Derivation of the FSF Approximations**

The approximations of neutron porosity and density measurements described in this paper are adapted from the extended Born approximation for the simulation of electromagnetic borehole measurements introduced by Torres-Verdín and Habashy (2001).

**Born Approximation.** An alternative form of Equation (A2) is given by

\[
\Phi(r_s,E) = \Phi_a(r_s,E) \left[1 + \frac{\Delta \Phi(r_s,E)}{\Phi_b(r_s,E)}\right],
\]

where

\[
\Delta \Phi(r_s,E) = \int_{E_l}^{E_u} dE \int_{\mathcal{S}} G(r_s,E \rightarrow r_s,E) \Phi_b(r_s,E) \frac{\Delta \Sigma(r_s,E)}{\Sigma_b(r_s,E)} \, dr_s,
\]

and

\[
\Phi_b(r_s,E) = \int_{E_l}^{E_u} dE \int_{\mathcal{S}} G(r_s,E \rightarrow r_s,E) \Phi_b(r_s,E) \, dr_s.
\]

The weighting function (spatial flux-scattering function of the source-detector response) is given by

\[
\Phi_b(r_s,E) = G(r_s,E \rightarrow r_s,E) \Phi_b(r_s,E),
\]

where the weighed parameter is \(\Delta \Sigma(r,E)/\Sigma_b(r,E)\).
Extended Born Approximation. We let \( r_s \in \mathcal{S} \). The particle flux at \( r \) is given by

\[
\Phi(r) = \int_{E_i}^{E_f} dE \Phi_\beta(r, E)
\]

\[
+ \int_{E_i}^{E_f} dE \int_{\mathcal{S}} G(r_s, E' \rightarrow r_s, E') \Phi_\beta(r_s, E') \frac{\Delta \Sigma(r_s, E)}{\Sigma_\beta(r_s, E)} dr_s.
\]

(B1)

On the other hand, the flux inside the scatterer region \( \Phi(r_0) \) is approximated with a Taylor series expansion centered at an observation point \( r \), as follows:

\[
\Phi(r_0) = \Phi(r) + (r_0 - r) \cdot \nabla \Phi(r)
\]

\[
+ \frac{1}{2} (r_0 - r) \cdot \nabla \nabla \Phi(r) \cdot (r_0 - r) + ...
\]

By retaining only the first term in the above expression, \( \Phi(r_0) \approx \Phi(r) \), one can explicitly solve for \( \Phi(r) \) as

\[
\Phi(r) \approx \Phi_\beta(r)
\]

\[
+ \Phi(r) \int_{E_i}^{E_f} dE \int_{\mathcal{S}} G(r_s, E' \rightarrow r_s, E') \frac{\Delta \Sigma(r_s, E)}{\Sigma_\beta(r_s, E)} dr_s,
\]

and

\[
\Phi_\beta(r) \approx \Phi(r)
\]

\[
\left[ 1 - \int_{E_i}^{E_f} dE \int_{\mathcal{S}} G(r_s, E' \rightarrow r_s, E') \frac{\Delta \Sigma(r_s, E)}{\Sigma_\beta(r_s, E)} dr_s \right],
\]

which yields

\[
\Phi(r) \approx \Phi_\beta(r) \frac{\Delta \Phi(r)}{D(r)}.
\]

where

\[
D(r) = 1 - \int_{E_i}^{E_f} dE \int_{\mathcal{S}} G(r_s, E' \rightarrow r_s, E') \frac{\Delta \Sigma(r_s, E)}{\Sigma_\beta(r_s, E)} dr_s.
\]

In the above expressions, \( \Phi(r) = \Phi_\beta(r) / D(r) \) constitutes the extended Born approximation for interior points. Further substitution of the above expression into Equation (B1), yields the extended Born approximation for exterior points, and is given by

\[
\Delta \Phi(r_s) \approx \int_{E_i}^{E_f} dE \int_{\mathcal{S}} G(r_s, E' \rightarrow r_s, E') \frac{\Phi_\beta(r_s, E') \Delta \Sigma(r_s, E)}{\Sigma_\beta(r_s, E)} dr_s.
\]

(B2)

Here, the flux-scattering function \( F_\beta \) is written as

\[
F_\beta(r_s, E) = G(r_s, E' \rightarrow r_s, E') \frac{\Phi_\beta(r_s, E)}{D(r_s, E)}.
\]

Alternative Formulation. For points inside the scatterer region, \( \mathcal{S} \), the flux at \( r \) is given by

\[
\Phi(r) = \Phi_\beta(r) \Upsilon(r), \text{ where } \Upsilon(r) \text{ is an auxiliary scattering function.}
\]

To find an approximation for \( \Upsilon(r) \), as in the case of \( \Phi(r) \), we consider a Taylor series expansion at an observation point \( r \in \mathcal{S} \), namely,

\[
\Phi(r_0) = \Phi_\beta(r_0) \Upsilon(r_0)
\]

\[
= \Phi_\beta(r_0) \left[ \Upsilon(r) + (r_0 - r) \right.
\]

\[
\cdot \Upsilon(r) + \frac{1}{2} (r_0 - r) \cdot \nabla \Upsilon(r_0 - r) + ...
\]

By retaining only the zeroth-order term of the above expression, one obtains

\[
\Phi(r_0) \Upsilon(r_0) \approx \Phi_\beta(r_0).
\]

Furthermore, by substituting this last expression back into Equation (B1) one obtains

\[
\Phi_\beta(r) \Upsilon(r) \equiv \Phi_\beta(r)
\]

\[
+ \Upsilon(r) \int_{E_i}^{E_f} dE \int_{\mathcal{S}} G(r_s, E' \rightarrow r_s, E') \Phi_\beta(r_s, E') \frac{\Delta \Sigma(r_s, E)}{\Sigma_\beta(r_s, E)} dr_s.
\]

and

\[
\Phi_\beta(r) \equiv \Upsilon(r) \left[ \Phi_\beta(r) - \int_{E_i}^{E_f} dE \int_{\mathcal{S}} G(r_s, E' \rightarrow r_s, E') \Phi_\beta(r_s, E') \frac{\Delta \Sigma(r_s, E)}{\Sigma_\beta(r_s, E)} dr_s \right].
\]

Solving for \( \Upsilon(r) \) yields

\[
\Upsilon(r) \approx \Phi_\beta(r) / D(r),
\]

where
whereupon the extended Born approximation for \( \Psi(r_x) \) is given by

\[
\Delta \Phi(r_x) = \int_{E_i}^{E_f} dE \int G(r_x, E \rightarrow r_x, E) \frac{\Phi_b(r_x, E)}{D(r_x, E)} \Delta \Sigma(r_x, E) \, dr_x,
\]

Consequently, the Flux-scattering function \( F_b \) is given by

\[
F_b(r_x, E) = G(r_x, E \rightarrow r_x, E) \frac{\Phi_b(r_x, E)}{D(r_x, E)}.
\]

**Rytov Approximation.** The assumption of \( \Delta \Phi(r_x, E) \propto \Phi_b(r_x, E) \) gives

\[
\ln \left[ \frac{\Phi(r_x, E)}{\Phi_b(r_x, E)} \right] - \ln \left[ \Phi_b(r_x, E) \right] \equiv \left( \frac{\Delta \Phi}{\Phi_b} \right) (r_x, E),
\]

or alternatively,

\[
\Phi(r_x, E) \approx \Phi_b(r_x, E) \exp \left( \frac{\Delta \Phi}{\Phi_b} (r_x, E) \right),
\]

where \( \Delta \Phi(r_x) \) is given by Equations (B2) and (B3).

**APPENDIX C: Practical Implementation of the FSF Approximations**

**Approximation for Density Measurements.** For the case of simulations of density measurements, the formation mass density is the weighted property.

Accordingly, let

\[
D(r) = \Phi_s(r) - \int_{E_i}^{E_f} dE \int G(r_x, E \rightarrow r_x, E) \Phi_b(r_x, E) \frac{\Delta \Sigma(r_x, E)}{\Sigma_b(r_x, E)} \, dr_x,
\]

and the Rytov approximation is given by

\[
\Phi(r_x) \equiv \Phi_b(r_x) \cdot \exp \left[ \frac{1}{\Phi_b(r_x)} \int_{E_i}^{E_f} dE \int F_b(r_x, E) \left( -C \rho \ln \left( \frac{\rho(r_x, E)}{\rho_b(r_x)} \right) \right) \, dr_x \right].
\]

In the above expressions, \( E_L \) and \( E_U \) are the corresponding lower and upper energy limits, respectively, for Compton scattering. The FSF is given by

\[
F_b(r_x, E) = G(r_x, E \rightarrow r_x, E) \Phi_b(r_x, E)
\]

for the Born approximation, and

\[
F_b(r_x, E) = G(r_x, E \rightarrow r_x, E) \frac{\Phi_b(r_x, E)}{D(r_x, E)}
\]

and

\[
F_b(r_x, E) = G(r_x, E \rightarrow r_x, E) \frac{\Phi_b(r_x, E)}{D(r_x, E)}
\]

for the extended Born approximations.

The flux measured at the detector is related to electron density by way of the expression

\[
\Phi(r_x) = A \exp(-B \rho_b),
\]

where \( A \) and \( B \) are calibration constants, and the bulk density is conventionally given by \( \rho = 1.0704 \rho_e - 0.1883 \), where \( \rho_e \) is electron density (Ellis, 1987).

**Approximation for Photoelectric-Factor Measurements.** For the case of simulations of PEF and U measurements, the formation U is the weighed property.

Accordingly, we let

\[
\frac{\Delta \Sigma(r)}{\Sigma_b(r)} = -C \rho \ln \left( \frac{U(r)}{U_b(r)} \right),
\]

whereupon the Born approximation takes the form

\[
\Phi(r_x) = \Phi_b(r_x) \cdot \exp \left[ \frac{1}{\Phi_b(r_x)} \int_{E_i}^{E_f} dE \int F_b(r_x, E) \left( -C \rho \ln \left( \frac{U(r_x)}{U_b(r_x)} \right) \right) \, dr_x \right],
\]

and the Rytov approximation is given by

\[
\Phi(r_x) = \Phi_b(r_x) \cdot \exp \left[ \frac{1}{\Phi_b(r_x)} \int_{E_i}^{E_f} dE \int F_b(r_x, E) \left( -C \rho \ln \left( \frac{U(r_x)}{U_b(r_x)} \right) \right) \, dr_x \right].
\]
\[
\Phi(r_s) \equiv \Phi_b(r_s)
\]
\[\exp \left[ \frac{1}{\Phi_b(r_s)} \int_{E_L}^{E_U} dE \int_{E_L}^{E_U} F_{\phi}(r_s, E) \left( -C_\phi \ln \left( \frac{U_b(r_s)}{U_b(r_s)} \right) \right) dE, \right] \]

(C4)

In the above expression, \(E_L\) and \(E_U\) are the lower and upper energy limits, respectively, of photoelectric factor measurements.

**Approximation for Neutron Measurements.** For the case of simulations of neutron measurements, the formation modified migration length is the weighed property.

Accordingly, we let

\[
\frac{\Delta \Sigma(r)}{\Sigma_b(r)} = -C_N \ln \left( \frac{L_{\text{neq}}(r)}{L_m(r)} \right),
\]

the Born approximation takes the form

\[
\Phi(r_s) \equiv \Phi_b(r_s)
\]
\[+ \int_{E_L}^{E_U} dE \int_{E_L}^{E_U} F_{\phi}(r_s, E) \left( -C_\phi \ln \left( \frac{L_{\text{neq}}(r_s)}{L_m(r_s)} \right) \right) dE, \]

(C5)

and the Rytov approximation is given by

\[
\Phi(r_s) \equiv \Phi_b(r_s) \frac{1}{\Phi_b(r_s)} \int_{E_L}^{E_U} dE \int_{E_L}^{E_U} F_{\phi}(r_s, E) \left( -C_\phi \ln \left( \frac{L_{\text{neq}}(r_s)}{L_m(r_s)} \right) \right) dE, \]

(C6)

In the above expressions, the energy limits \(E_L\) and \(E_U\) include the thermal and epithermal neutron energy. Because of its dependence on \(\Sigma\), the appropriate weighed property for describing the response of thermal neutron measurements is the modified migration length, \(L'_m\), given by (Ellis et al. 1987; McKeon et al. 1989; Kreft, 1974)

\[
L'_m = \sqrt{L^2 + g(L_s) L^2_{s}},
\]

and

\[
g(L_s) = a\sqrt{L_s} - b,
\]

where \(L_s\) is the slowing-down length and \(L_s\) is the diffusion length.

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